

First LBNL Projects Included in Latest Globus Toolkit

The latest version of the Globus Toolkit, GT3.2, contains pyGlobus and pyGridWare, two components developed as DOE-funded projects by members of the Secure Grid Technologies Group in CRD's Distributed Systems Department. This marks the first inclusion of Berkeley Lab projects in the toolkit, the latest version of which was released Feb. 16, 2004.

"I was very pleased to have our efforts included," said Keith Jackson, leader of the project. "Now there is a much larger group of users who can benefit from our efforts to make the Grid easier to use."

PyGlobus provides an easier, cleaner, high-level interface to the Globus Toolkit, making the various Grid tools easier to use, Jackson said. The group uses the Python programming language because it utilizes simple, clean syntax and is widely used by the scientific community.

PyGridWare is the Python-based implementation of OGSi, the Open Grid Services Infrastructure. It provides client tooling to support automatically generating bindings to OGSi services, and is fully interoperable with the Java OGSi implementation from Argonne National Lab and IBM.

Getting the two projects included in the toolkit required that the developers demonstrate an existing user base, show that the applications were of sufficient quality, and provide ongoing support. The group will also update both pyGridWare and pyGlobus as new versions of the Globus Toolkit are developed and released.

For more information, contact Keith Jackson at KRJackson@lbl.gov or go to <http://www-itg.lbl.gov/SGT/>.

What is CRD Report?

This is the second issue of CRD Report, a publication highlighting recent achievements by staff members in Berkeley Lab's Computational Research Division. Initially, CRD Report will be distributed every other month via email and posted on the Web at <http://crd.lbl.gov/DOEResources>, and may be freely distributed. CRD Report is edited by Jon Bashor, JBashor@lbl.gov or 510-486-5849.

CRD's AMR Methods Accelerate MHD Simulations

The annual Supercomputing conference held every November is well known as a sort of international watering hole, where many of the world's leading experts in high-performance computing gather for a week to take stock of the competition, exchange ideas, and make new connections.

At SC2000 in Dallas, Phil Colella, head of the Applied Numerical Algorithms Group at Lawrence Berkeley National Laboratory, and Steve Jardin, co-leader of the Computational Plasma Physics Group at Princeton Plasma Physics Laboratory, were both scheduled to give talks in the Berkeley Lab booth. Colella discussed "Adaptive Mesh Refinement Research and Software at NERSC," where Jardin has conducted his scientific computing for years. Jardin gave a presentation on "A Parallel Resistive MHD Program with Application to Magnetic Reconnection."

The scientist and the mathematician got to talking between their presentations and one thing led to another. They began an informal collaboration which was soon formalized under the auspices of SciDAC—Jardin is principal investigator for the Center for Extended Magnetohydrodynamic Modeling

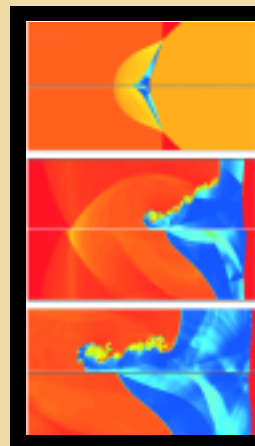


Figure 1. Stabilization of Richtmyer-Meshkov instability by a magnetic field. From R. Samtaney, "Suppression of the Richtmyer-Meshkov instability in the presence of a magnetic field," Princeton Plasma Physics Laboratory report PPPL-3794 (submitted to Phys. Fluids).

(CEMM), while Colella is PI for the Applied Partial Differential Equations Center (APDEC). Jardin's group was able to incorporate the CHOMBO adaptive mesh refinement (AMR) code developed by Colella's group into a new fusion simulation code, which is now called the Princeton AMRMHD code. "Using the AMR code resulted in a 30 times improvement over what we would have had with a uniform mesh code of the highest resolution," Jardin says.

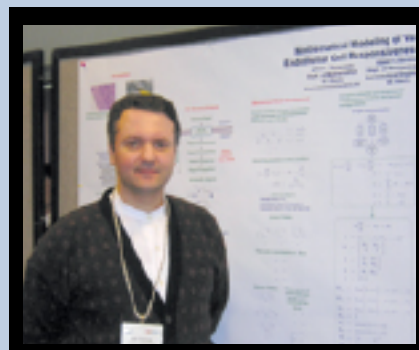
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Lab Hosts 85 Researchers at Fifth Bay Area Scientific Computing Day

Eighty-five researchers in computational science and engineering turned out for the Fifth Bay Area Scientific Computing Day held Saturday, March 13, at Berkeley Lab. The meeting is an informal gathering to encourage the interaction and collaboration of researchers in the San Francisco Bay Area.

The annual event provides a venue for junior researchers to present their work to the local community, and for the Bay Area scientific computing and computational science communities to exchange views on today's multidisciplinary computational challenges and state-of-the-art developments. The program included technical talks, a roundtable discussion and poster presentations.

Among those attending was Alan Laub, head



John Tamaresis of UC Davis, who presented a poster during the program, said he found the event very worthwhile.

of DOE's Scientific Discovery through Advanced Computing and former dean of Engineering at UC Davis, who called the meeting "very valuable."

"The scientists assembled here today represent teams of people from three major fields — math, computer science and applications,"

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Laub said. "People from different fields have the opportunity to get together and learn ideas from each other, all on a local scale. It's great listening to the young people in the various fields because you realize that these are the scientists of the future."

John Tamaresis, a math student at UC Davis who presented a poster, said the event had much to recommend it, including "the variety and quality of the presentations and posters, Phil Colella's enthusiasm for the subject of my poster, a lively discussion about training computational scientists, and deep insights offered to me by Professor Kahan of UC Berkeley."



Rob Schreiber (left) of HP and Alan Laub of DOE and UC Davis relax during the lunch break.

The attendees came from industry, research labs and universities. Those represented

include Hewlett Packard, Polymath Research Inc., Visual Numerics, LBNL, LLNL, NASA Ames Research Center, Sandia National Laboratories, Stanford Linear Accelerator Center, UC Berkeley, UC Davis, University of San Francisco, UC San Francisco, San Francisco State University, Stanford University, Sonoma State University, Santa Clara University, San Jose State University and St. Mary's College.

The event was organized by Tony Drummond, Parry Husbands, Sherry Li and Osni Marques of the Scientific Computing Group in the Computational Research Division.

Fusion (continued from p.1)

The AMRMHD code, developed in conjunction with Princeton researcher Ravi Samtaney and Berkeley Lab researcher Terry Ligocki, is already producing new physics results as well. It powered the first simulation demonstrating that the presence of a magnetic field will suppress the growth of the Richtmyer-Meshkov instability when a shock wave interacts with a contact discontinuity separating ionized gases of different densities. The upper and lower images in Figure 1 contrast the interface without (upper) and with (lower) the magnetic field. In the presence of the field, the vorticity generated at the interface is transported away by the fast and slow MHD shocks, removing the driver of the instability. Results are shown for an effective mesh of $16,384 \times 2,048$ points which took approximately 150 hours to run on 64 processors of Seaborg—25 times faster than a non-AMR code.

Another new physical effect discovered by the AMRMHD code is current bunching and ejection during magnetic reconnection (Figure 2). Magnetic reconnection refers to the breaking and reconnecting of oppositely directed magnetic field lines in a plasma. In the process, magnetic field energy is converted to plasma kinetic and thermal energy.

The CEMM project has been collaborating with other SciDAC software centers in addition to APDEC. For example, in a collabora-

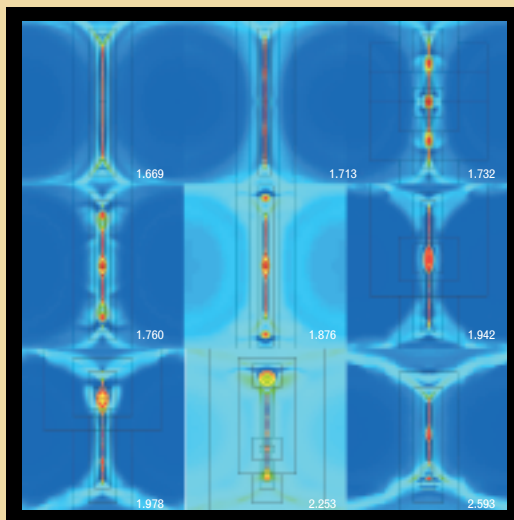


Figure 2. Current bunching and ejection during magnetic reconnection. From R. Samtaney, S. Jardin, P. Colella, and T. Ligocki, "Numerical simulations of magnetic reconnection using AMR," Sherwood Fusion Theory Conference, Rochester, NY, April 2002.

tion that predated SciDAC, the group developing the M3D code was using PETSc, a portable toolkit of sparse solvers distributed as part of the ACTS Collection of DOE-developed software tools. Also in the ACTS Collection is Hypre, a library of preconditioners that can be used in conjunction with PETSc. Under SciDAC, the Terascale Optimal PDE Solvers (TOPS) Center worked with CEMM to add Hypre underneath the same code interface that M3D was already

using to call the PETSc solvers. The combined PETSc-Hypre solver library allows M3D to solve its linear systems two to three times faster than before.

According to Jardin, fusion plasma models are continually being improved both by more complete descriptions of the physical processes, and by more efficient algorithms, such as those provided by PETSc and CHOMBO. Advances such as these have complemented increases in computer hardware speeds to provide a capability today that is vastly improved over what was possible 30 years ago. This rate of increase of effective capability is essential to meet the anticipated modeling demands of fusion energy research, Jardin says.

"Presently, we can apply our most complete computational models to realistically simulate both nonlinear macroscopic stability and microscopic turbulent transport in the smaller fusion experiments that exist today, at least for short times," Jardin says. "Anticipated increases in both hardware and algorithms during the next five to ten years will enable application of even more advanced models to the largest present-day experiments and to the proposed burning plasma experiments such as ITER [the International Thermonuclear Experimental Reactor]."

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